Argonne NATIONAL LABORATORY

... for a brighter future

A Vision for the Renewal of the Advanced Photon Source

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U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science U.S. DEPARTMENT OF ENERGY

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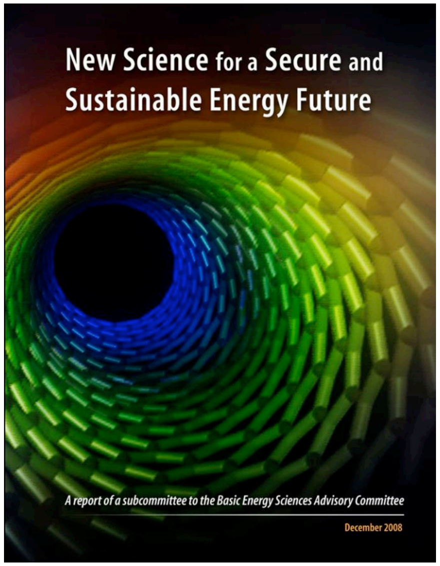
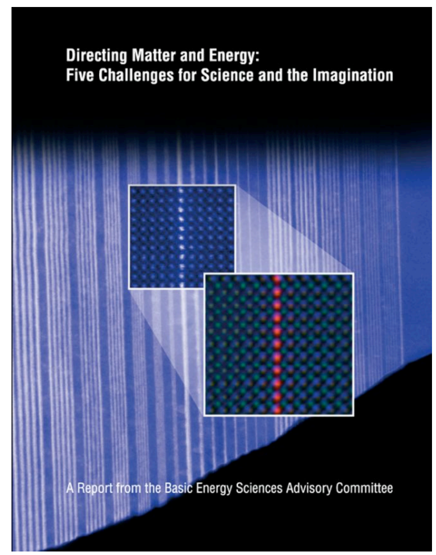
What are the scientific grand challenges?



How do we control material processes at the level of electrons?
How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?
How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
How do we characterize and control matter away— especially very far away —from equilibrium?

Materials with Unprecedented Performance
Making Chemical Change More Selective
Returning Carbon to the Earth
Safer and More Efficient Nuclear Power
Let There Be (Digital) Light
A Solar Economy for Buildings 6
A Hybrid Electrical Grid
Advanced Transport
Solar Fuels
Electric Transport



Many of these challenges demand hard x-rays with higher spatial and temporal resolution… APS wants to deliver the best for decades to come

- APS is the brightest source of hard x-rays for the next decade in North America
- Hard x-rays have unique capabilities in addressing the grand challenges
  - Complex systems, extreme environments, …
- APS plans to remain at the forefront of hard x-ray science
  - The Renewal is a key step for the next decade
    - *Can deliver orders of magnitude better performance to expts*
  - We are also looking beyond the renewal to a 4th generation source
    - *transformational*

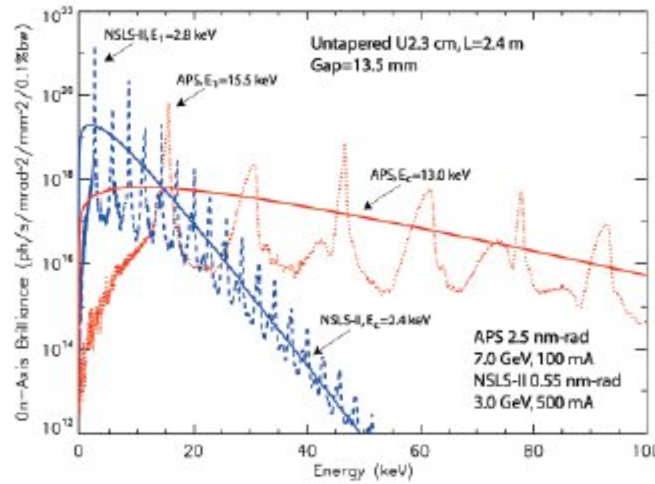
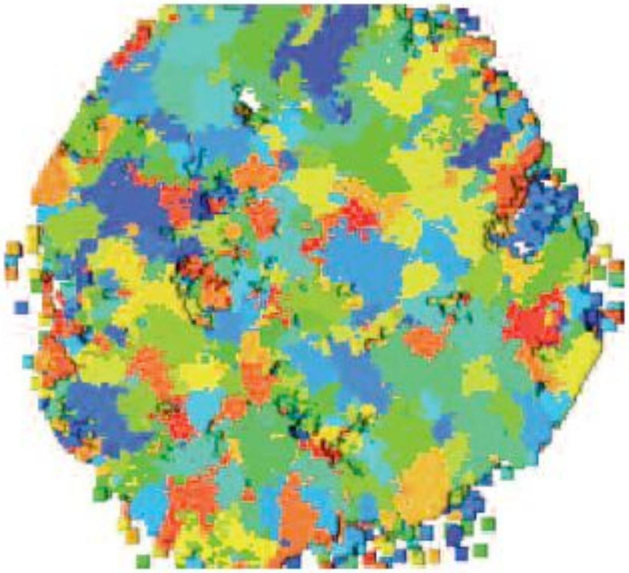
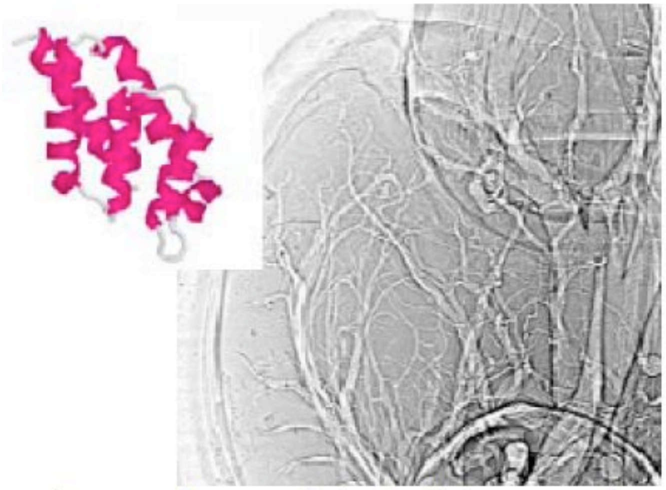


Fig. 1. On-axis brilliance for the untapered undulator U2.3 cm (APS23#1) installed on the APS and the NSLS-II storage rings. The undulator is 2.4-m long and the undulator gap is 13.5 mm. The first harmonics and the critical energies for two cases are labeled. The solid lines show the wiggler approximation using the corresponding critical energies. (Courtesy R. Dejus, Argonne National Laboratory)

Mastering Hierarchical Structures Through X-Ray Imaging



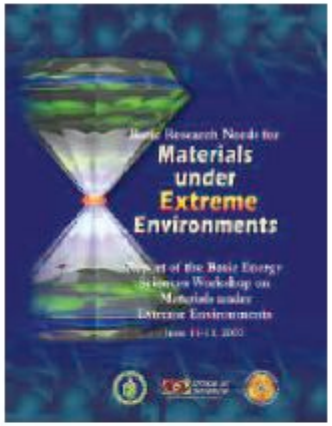
Three-dimensional distribution of grains in a 1-mm cube of aluminum. (Courtesy R. Suter et al., Carnegie Mellon University)



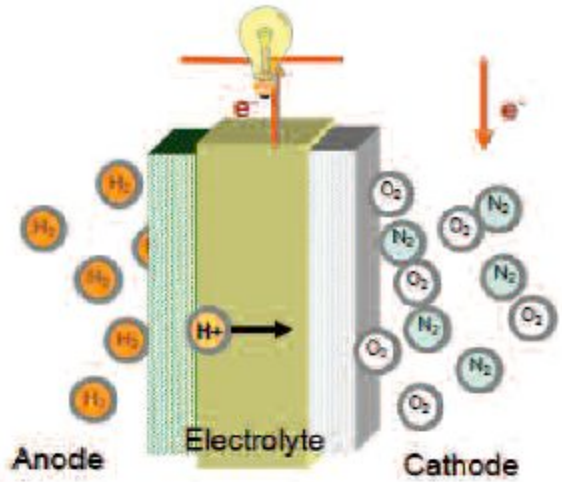
Images from proteins to living organisms will help connect the dots in understanding how genetics controls health and disease (image courtesy W.K. Lee)

- How can we make stronger, lightweight materials?
- How do we control the transport of environmental contaminants and store CO_2 in rock?
- How do we make clean biofuels from renewable ligno-cellulose?
- How do proteins fit together to make organisms?

Real materials in real conditions in real time



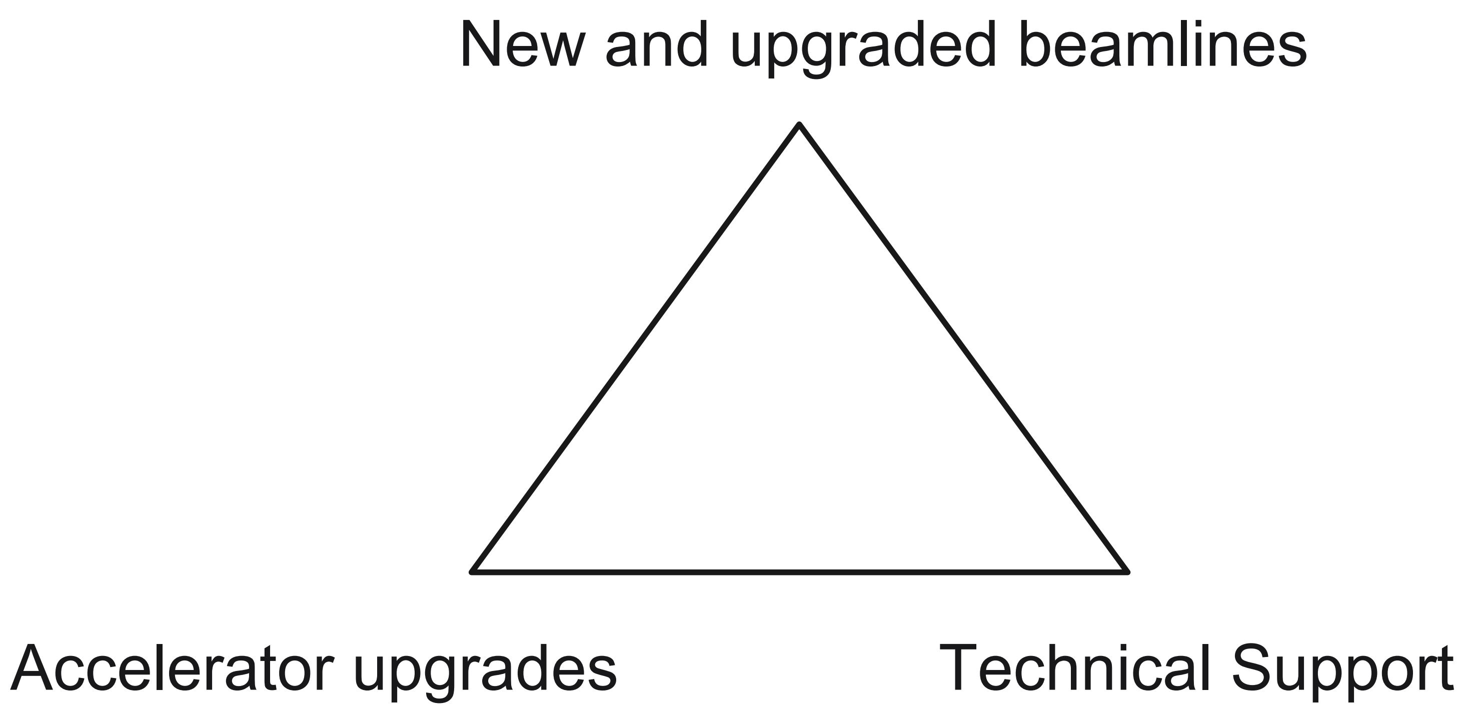
The cover of this BESAC report shows a diamond anvil cell. APS is a world-leader in high-pressure research.



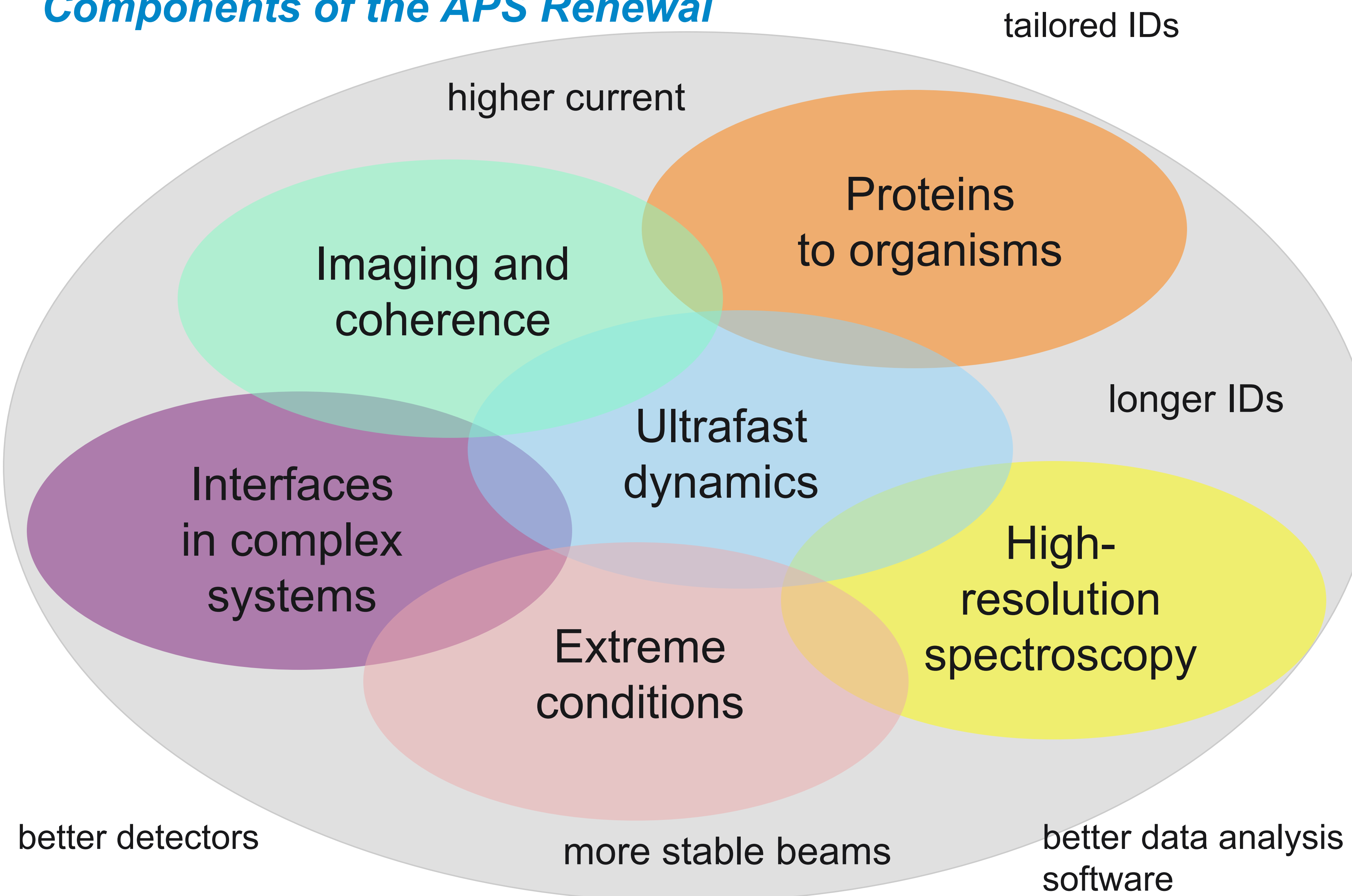
Schematic of an H_2 fuel cell. (Courtesy D. Myers, Argonne National Laboratory)

- How can we get the specificity of enzymes in catalysts?
- How can we load a battery efficiently with mobile ions to improve power/weight ratio?
- Can we imitate photosynthesis?
- How do we manufacture efficient lighting cost-effectively?
- Can we control nucleation to make better smarter materials?
- Can we develop new superconductors for the electric grid?

Key components of the Renewal



Components of the APS Renewal



Key components to execute this vision

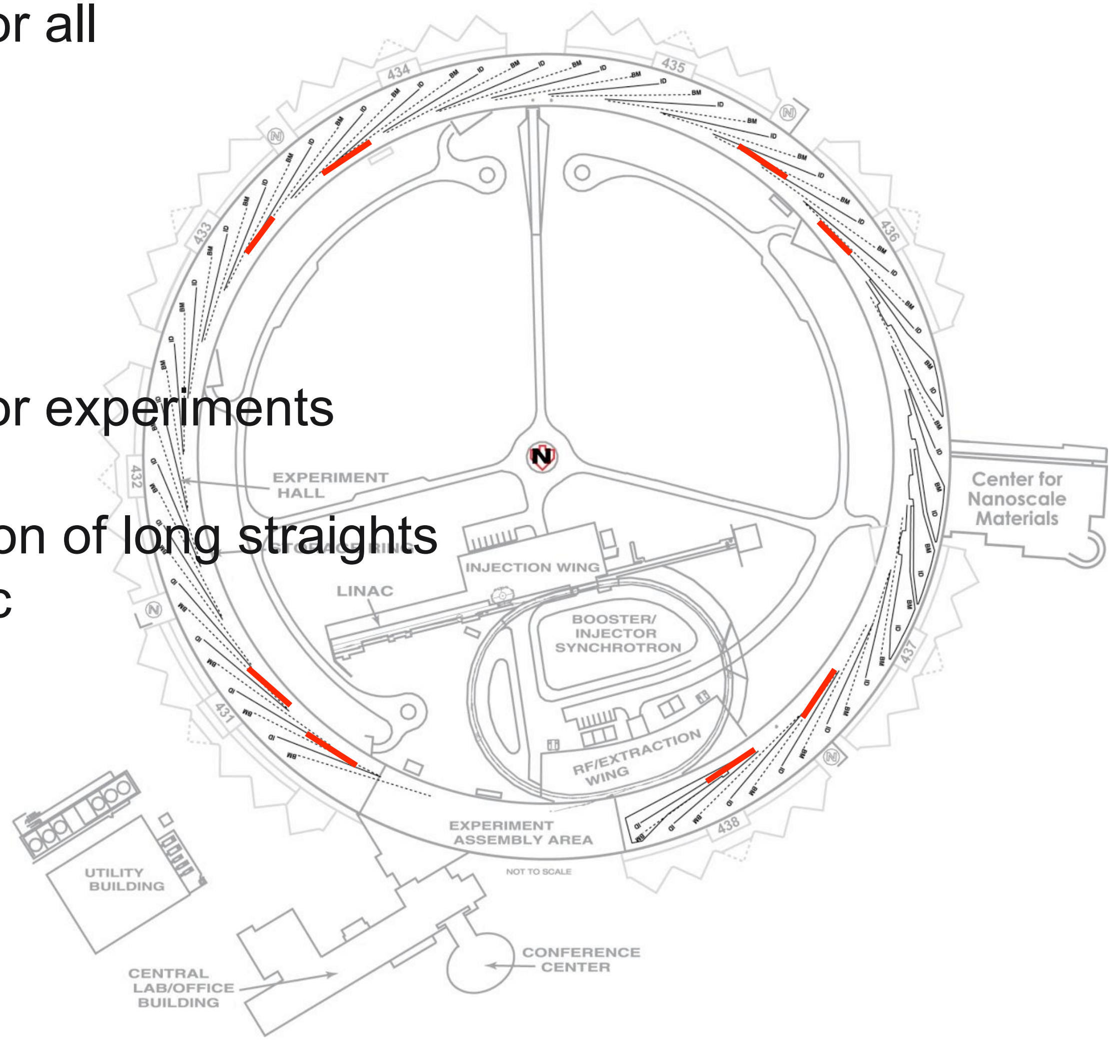
- Accelerator upgrades
  - Lattice with long straight sections
  - Tailored insertion devices
  - Higher current
  - Improved stability and optics
- New and upgraded beamlines
  - Imaging and coherence
  - Extreme conditions
  - Dynamics - From fast to ultra-fast
  - More sensitive spectroscopy
  - Interface science
  - Life science
- Technical support
  - Detectors
  - Computers and software
  - Infrastructure

Underlying is a new accelerator lattice with 8 x 8m straight sections, 200mA current and more stable beams

Optics and FEs for all beamlines
will be modified
to take advantage

Many new IDs
better optimized for experiments

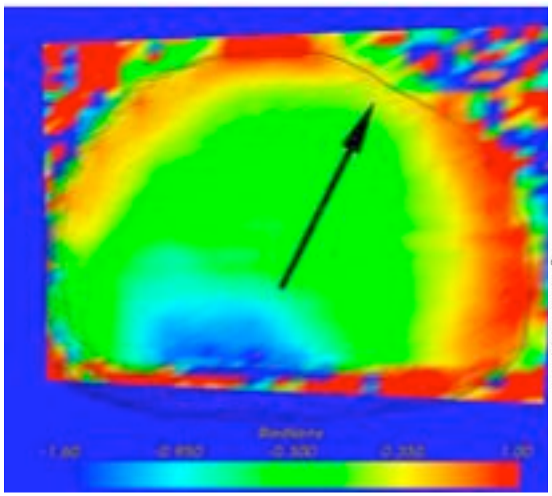
Flexibility in location of long straights
- provided periodic



Imaging and coherence– the challenges

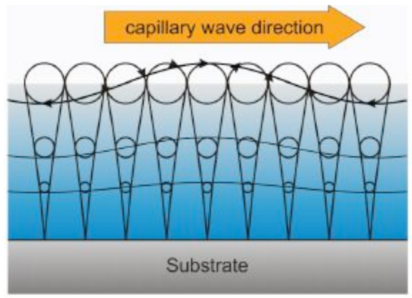
- We need to image light and heavy elements, in complex 3-D objects

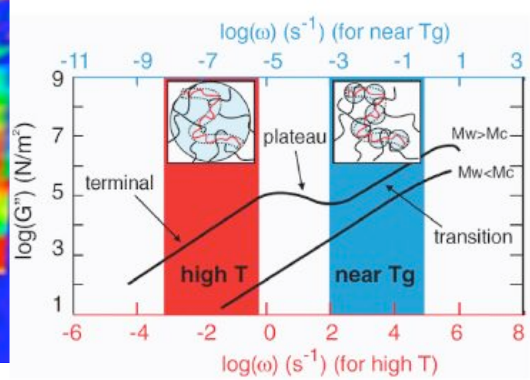
CDI of strain fields in nanostructures



R. Harder et. al. Phys. Rev. B 76, 115425 (2007)

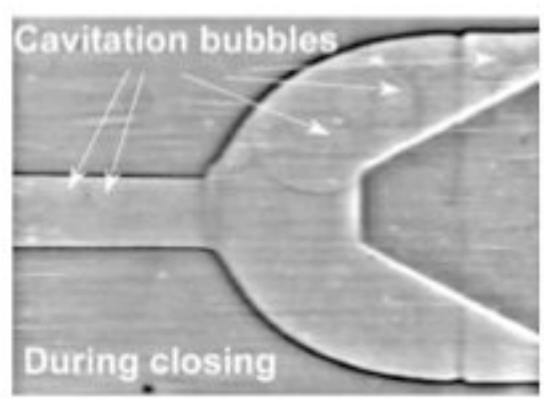
Polymer dynamics





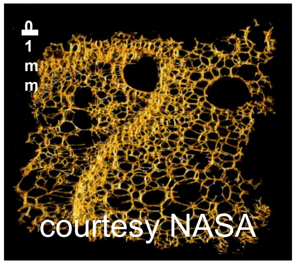
Jiang et. al. Phys Rev Lett. **101**, 246104 (2008)

Fast moving liquids

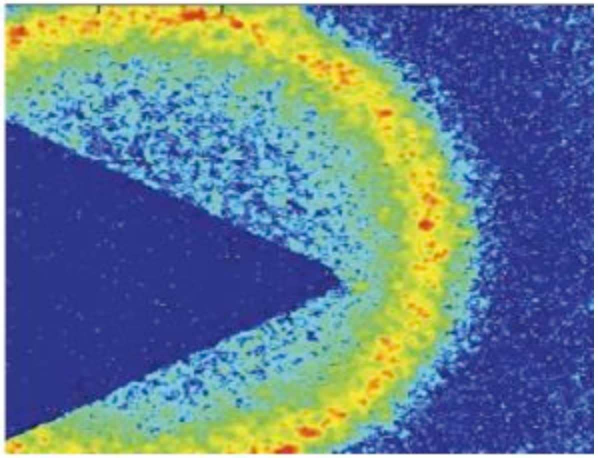


with large coherent field-of-view…

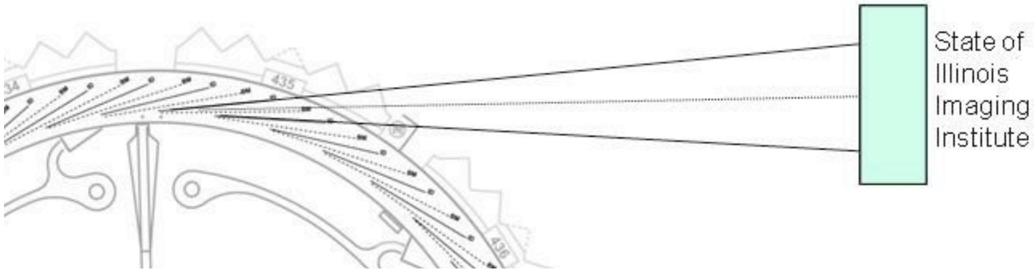
Imaging and coherence– new and upgraded beamlines



- Further dedicated imaging capability for tomography and phase contrast imaging (including bending magnets)
- Improved capability for XPCS
  increased coherent flux
  μs detector (with BNL)

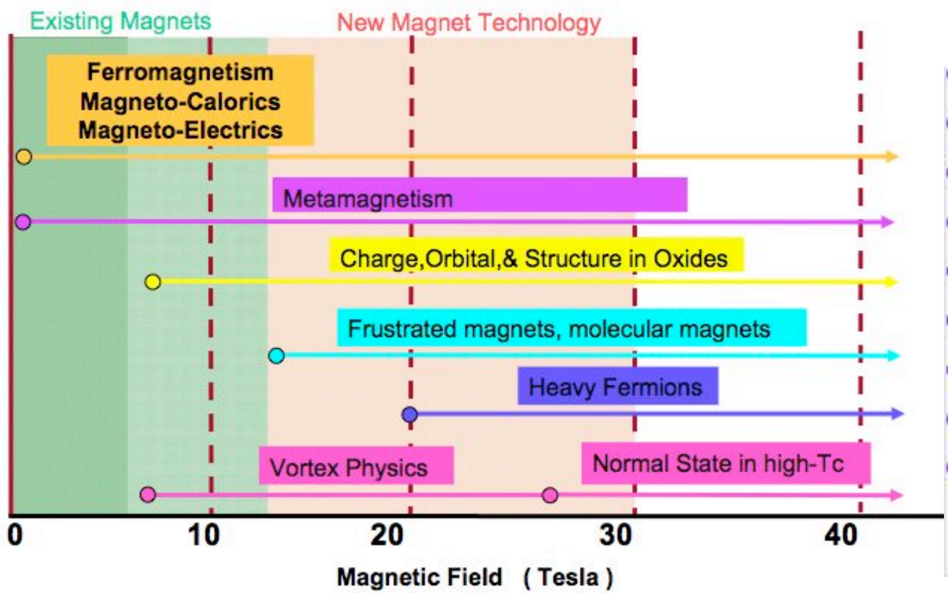


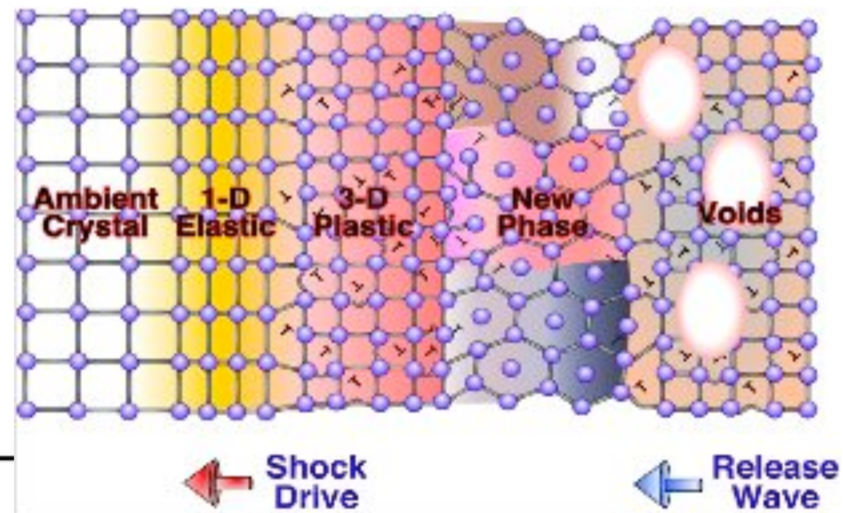
Long imaging beamline(s) for phase contrast imaging and CDI



Advanced x-ray imaging beamlines

Extreme conditions – the challenges

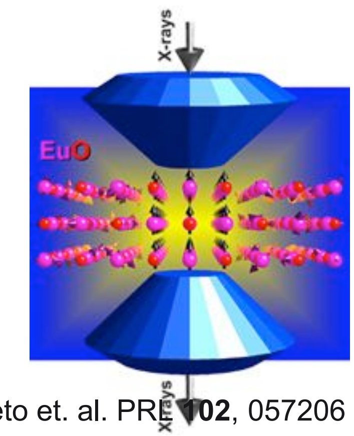




new materials

To go where no earth material has gone before..

Ma et. al., Nature 458, 182 (2009).

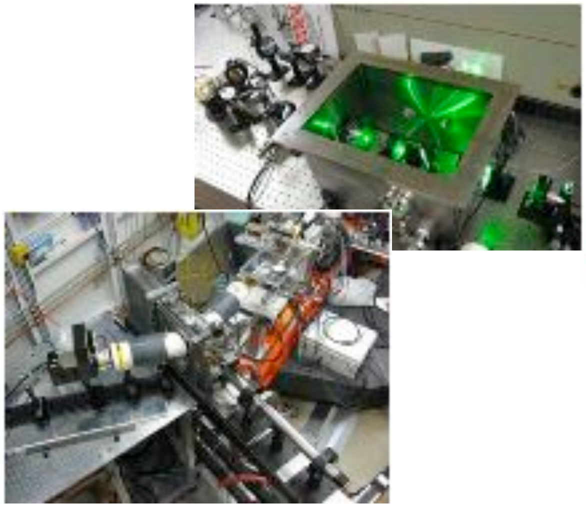


Increasing pressure ?

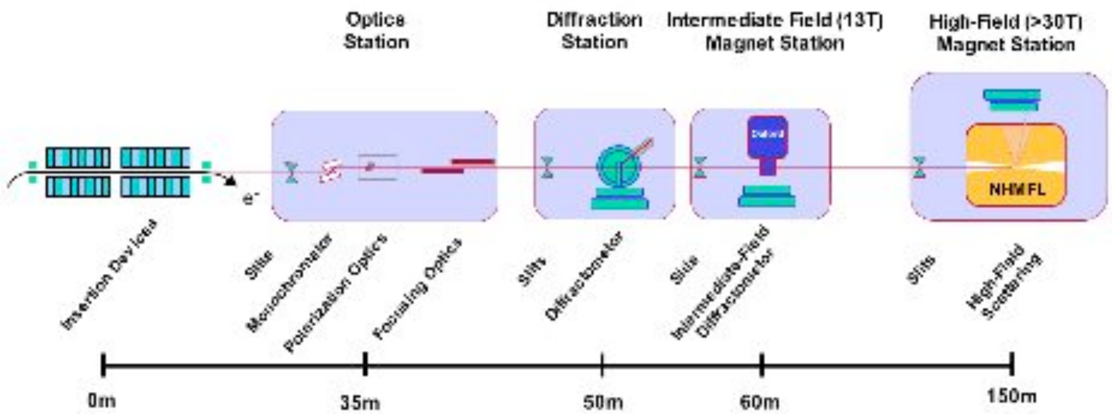
Souza-Neto et. al. PRL **102**, 057206 (2009)

Extreme conditions – new and upgraded beamlines

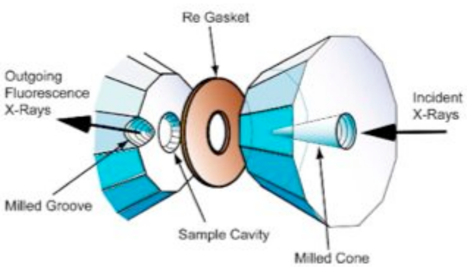
Dynamic Shock Compression BL
(DOE-NNSA)



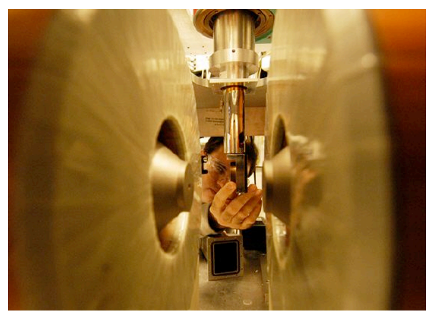
High Magnetic Field BL
(with NSF NHMFL)



expansion of HP-sync
multiple extreme environments



[Mayanovic *et al* Rev Sci Inst. 78, 053904 (2007)]



- Upgrades to HPCAT and GSE CARS

Ultrafast dynamics – the challenge

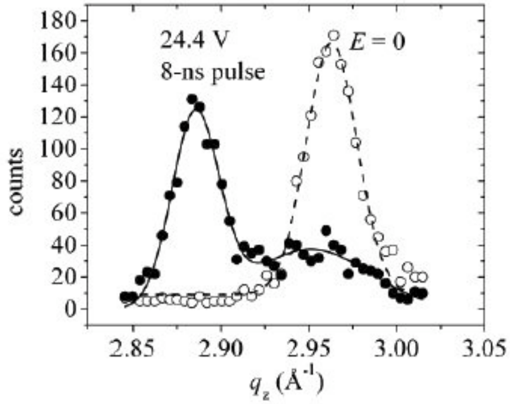
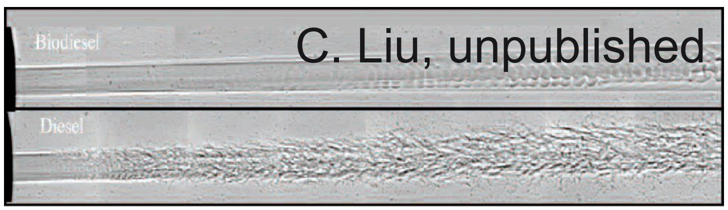


Fig. 4. Transient strain of 2.7% in a 40-nm-thick PZT film in response to an 8-ns electric-field pulse [26]. (© 2008 The American Physical Society)



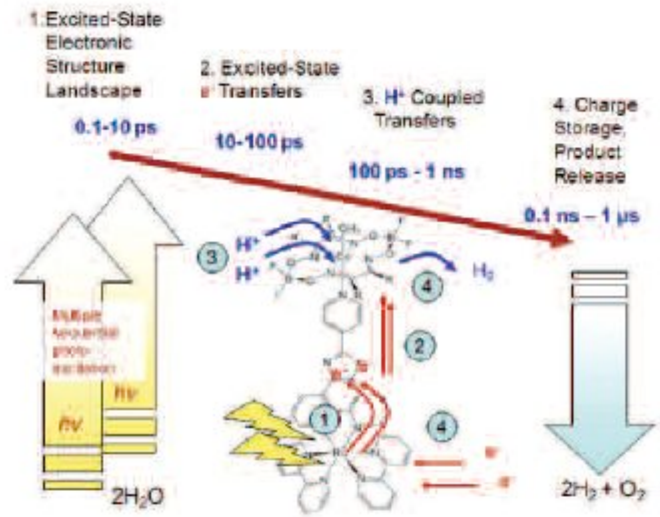
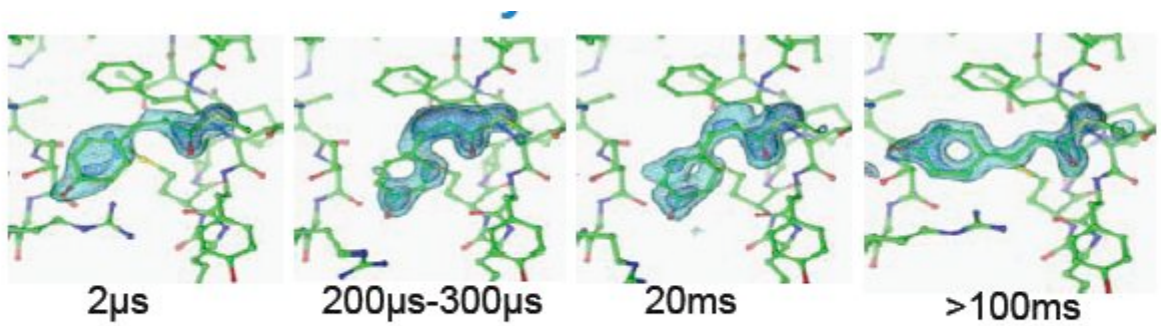


Fig. 7. Excited-state reaction cycle for a photosensitizer linked to a hydrogen-evolving catalyst. Prototype photocatalyst adapted from Fontcave et al., Angew. Chem. Int. Ed. **47**, 564 (2008). (Courtesy D. Tiede, Argonne National Laboratory)

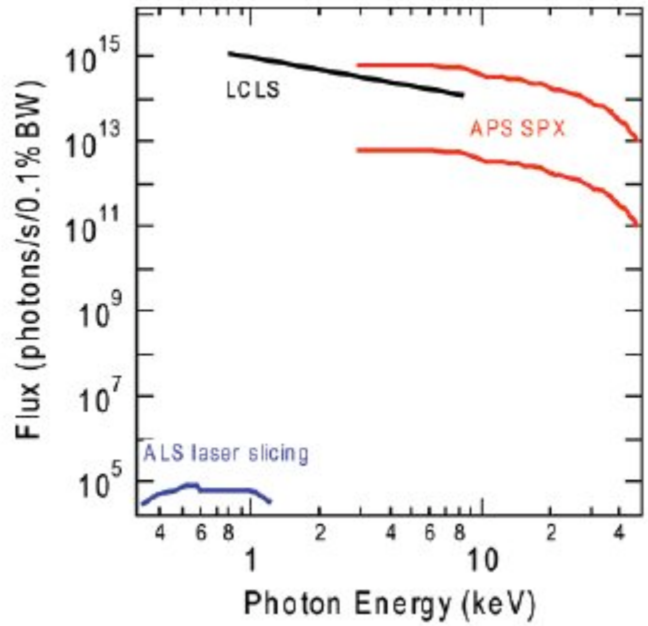
Vukica Srajer



Ultrafast dynamics – new and upgraded beamlines

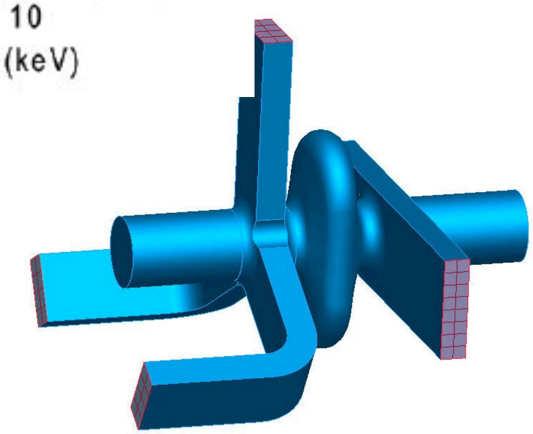
Pulse slicing source (1 or 2 sectors)

Wang et. al. PRL **100**, 154502 (2008)

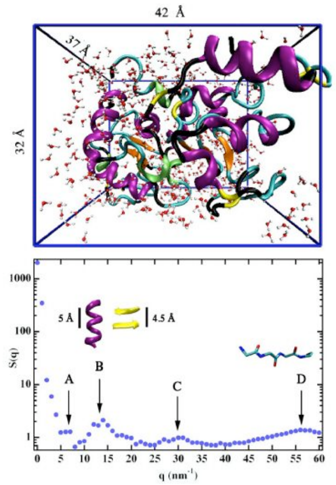


High speed GISAXS
and imaging

Preserve 24 bunch mode with higher current



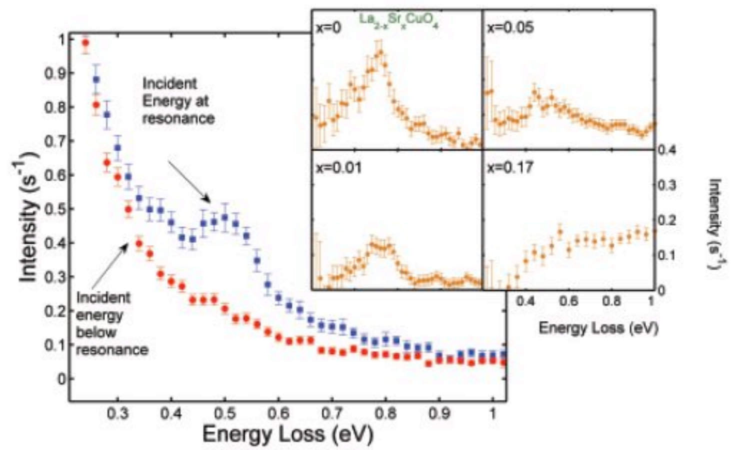
High-resolution spectroscopy – the challenge



Dynamics and protein function

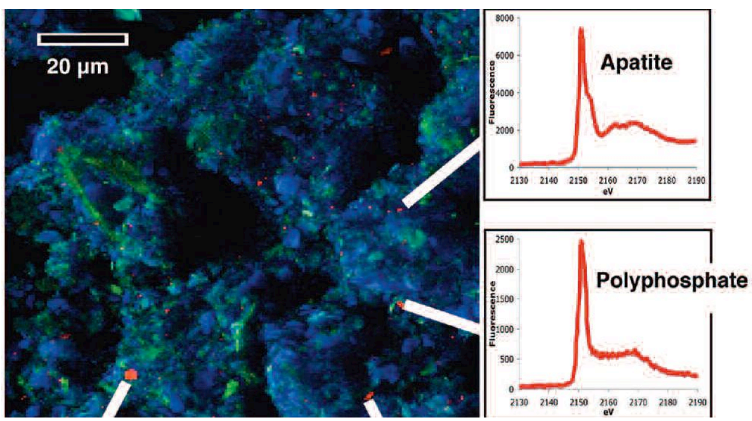
Liu et. al. PRL **101** 135501 (2008)

Collective excitations in superconductors



Hill et al., Phys. Rev. Lett. **100**, 097001 (2008)

Imaging elemental and chemical distributions



Demands higher spatial and energy resolution, higher signal…

High-resolution spectroscopy – new and upgraded beamlines

- HERIX and MERIX with dedicated beamlines and undulators (long straight)
- LERIX capability expanded
- Better spectroscopic detectors
- Dedicated micro-spectroscopy beamlines

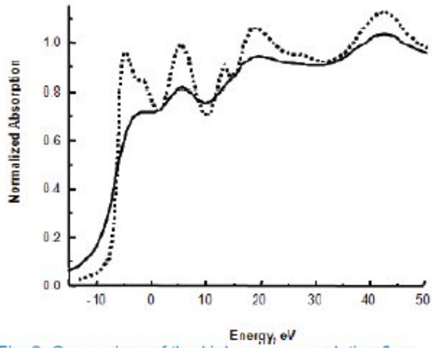


Fig. 2. Comparison of the high-energy-resolution fluorescence XANES (dotted) to the transmission XANES (solid) for Au foil [15]. (© 2006 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim)

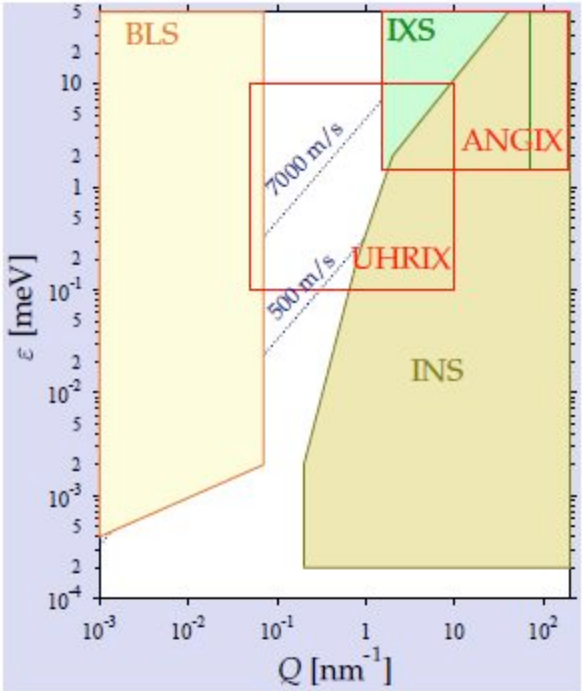
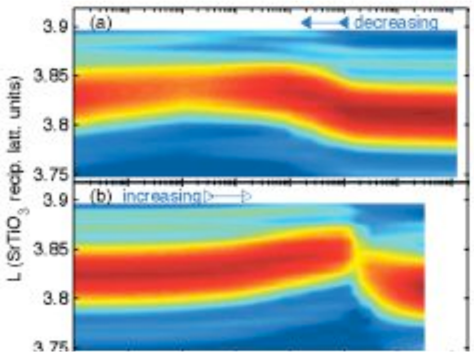


Figure 1: Existing techniques and proposed spectrometers mapped onto the energy ε and momentum transfer Q space.

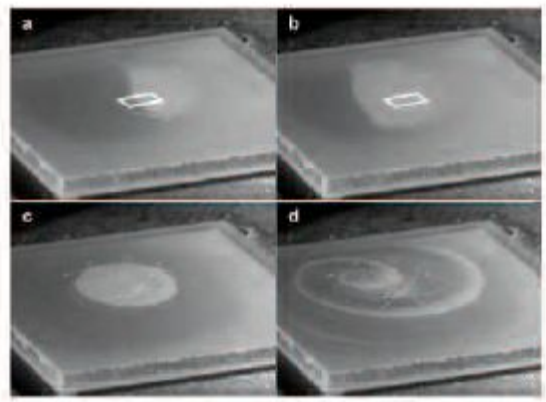
Interfaces in complex systems – the challenges

Chemical switching of ferroelectrics

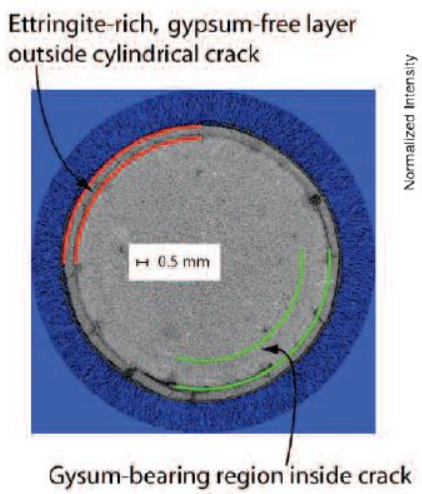


Wang, et al., Phys Rev Lett **102**, 047601 (2009)

Spatiotemporal instabilities for InN growth



Jiang et al., Phys. Rev. Lett. **101,** 086102 (2008)



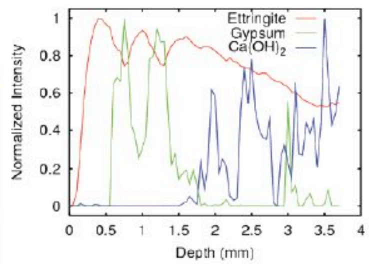
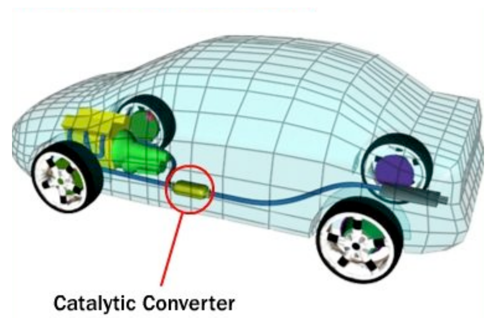


Fig. 6. Left: Microtomograph of a cement paste cylinder that has been exposed to sulfate solution showing subsurface crack formation. The corresponding depth profile for some of the crystalline phases in the same specimen, generated from energy dispersive x-ray diffraction data, is shown above. (Courtesy A. Wilkinson, Georgia Institute of Technology)



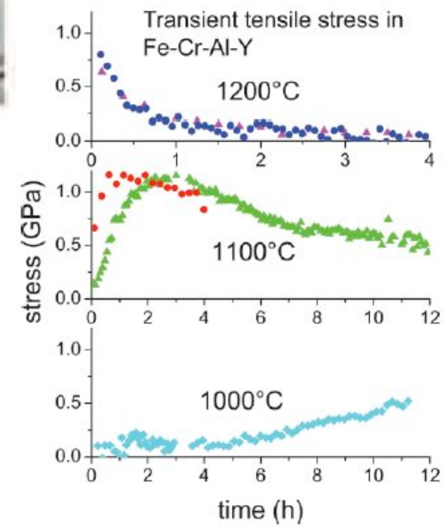


Fig. 3. Oxide stresses in a high-temperature steel at temperature. Because the lattice expands during oxidation, the oxide coating was assumed to be under compressive load. *In situ* experiments at the APS found that the coating is actually in tension, which is critical for cracking and failure of the protective oxide coating. (Courtesy E. Specht, Oak Ridge National Laboratory)

Interfaces in complex systems – new and upgraded beamlines

- New dedicated sector for X-ray Interfacial Scattering
  - Complementing endstations and increasing capacity
- Improved high-energy capabilities
- Catalysis beamline and other optimized endstations and instrumentation

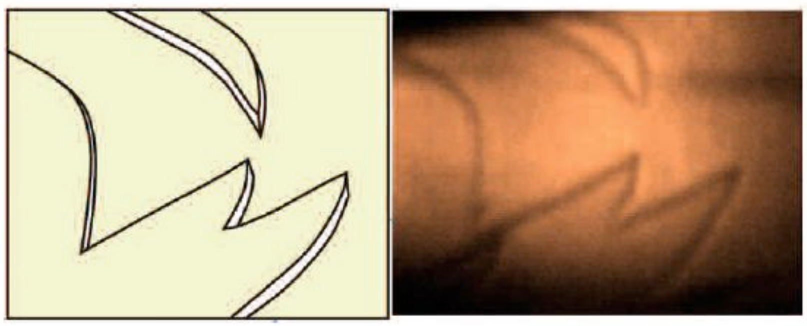


Fig. 5. The XRIM images elementary interfacial topography through intensity contrast. Left: Schematic interface topography. Right: An XRIM image where dark lines are 0.6-nm-high steps. (Fenter et al., Nat. Phys. **2**, 700 [2006], © 2006 Nature Publishing Group, a division of Macmillan Publishers Limited, all rights reserved)

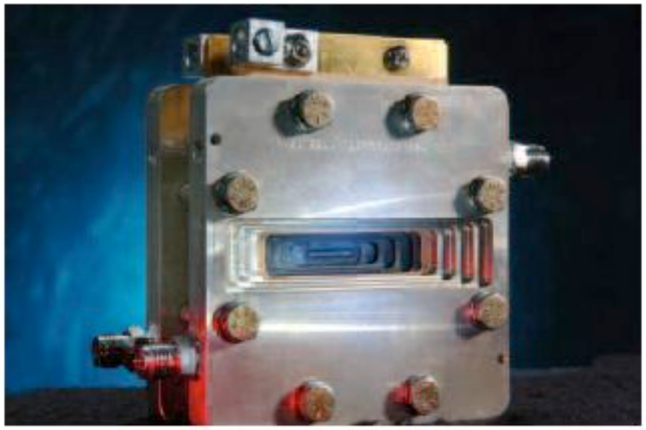


Fig. 4. Cell for *in situ* x-ray absorption studies of fuel cell catalysts. Standard Fuel Cell Technologies cell hardware was machined to allow x-ray fluorescence studies of cathode electrocatalysts in an operating membrane-electrode assembly (fuel cell). (Argonne National Laboratory photograph)

Connecting proteins to organisms – the challenge

- Proteins which are hard to crystallize (e.g. for neuropharmacology)
- Protein dynamics
- Proteins to organisms

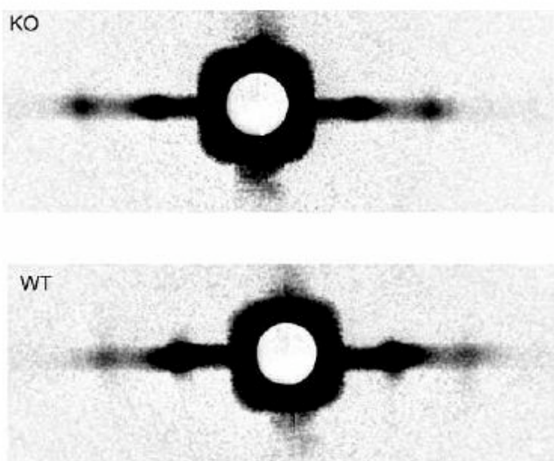


Fig. 3. X-ray diffraction patterns of normal mouse heart muscle (WT, bottom) and heart muscle from mice lacking cardiac myosin-binding protein-C (KO, top). Compared with WT muscle, the KO muscle matter is shifted toward its thin actin filaments (represented by the size of the outermost black dots in both images), as opposed to its thick myosin filaments (inner dots), implying that cardiac myosin-binding protein-C helps keep myosin filaments more tightly wound than they would be otherwise. (From: "Deconstructing Heart Muscle," *APS Science 2007*, ANL-07/25 [Argonne National Laboratory, May 2008] p. 66. Courtesy B. A. Colson, T. Bekyarova, D.P. Fitzsimons, T.C. Irving, and R.L. Moss. Imaged at Bio-CAT beamline 18-ID at the APS.)

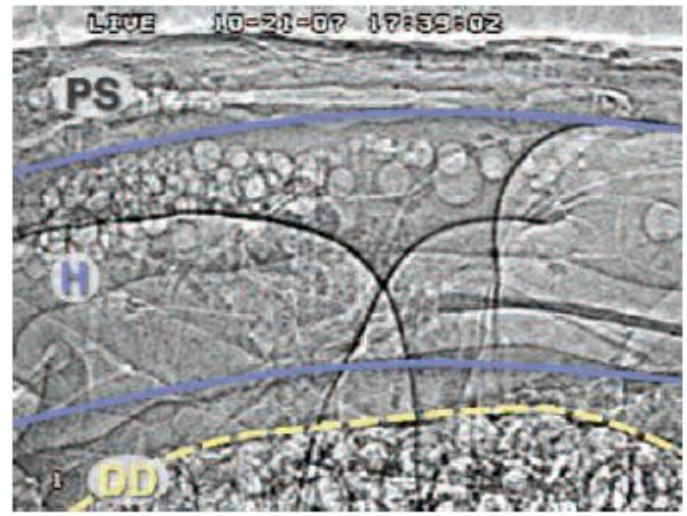
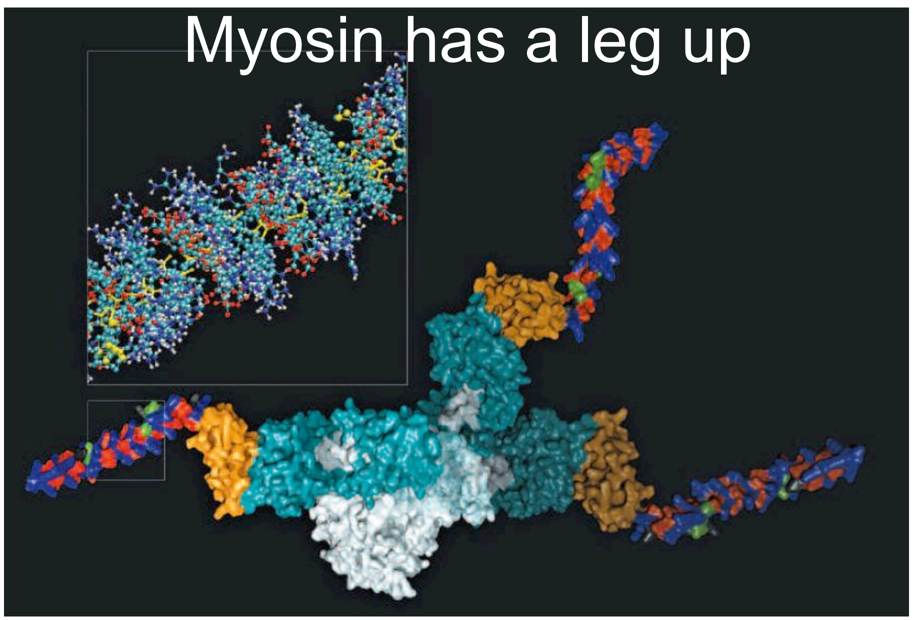


Fig. 1. From an x-ray video of flow visualization in the heart of a grasshopper (*Schistocerca americana*) obtained at the X-ray Operations and Research (XOR) beamline 32-ID at the APS using synchrotron x-ray phase-contrast imaging. This still image shows a region in the dorsal 3rd abdominal segment. Round structures are air bubbles used to visualize patterns of heartbeat and hemolymph flow. (Courtesy W.-K. Lee [Argonne National Laboratory] and J.J. Socha [Virginia Polytechnic and State University])

Connecting proteins to organisms – new and upgraded beamlines

- More stable beam and sample holders for microcrystallography
- Better Pixel Array detectors to use the beam most efficiently
- Better SAXS capabilities
- Better imaging capabilities



Spink et. al. Nat. Struct. Biol. **15**, 591 (2008)

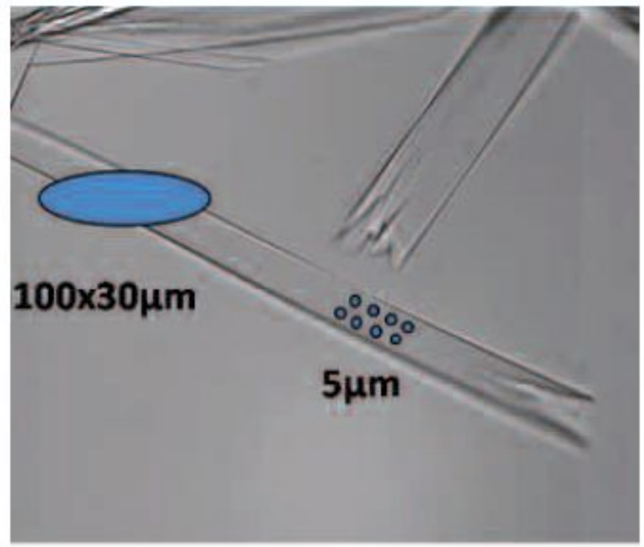
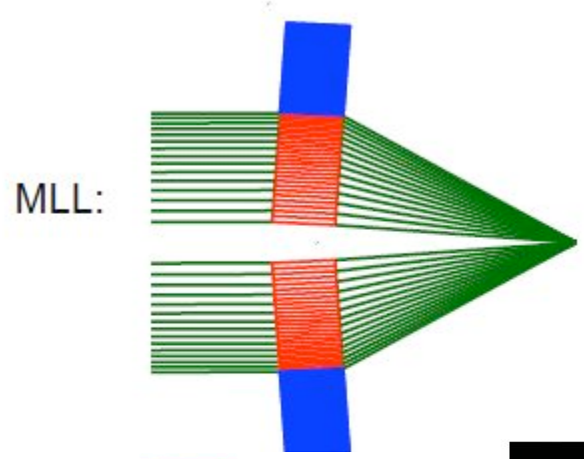
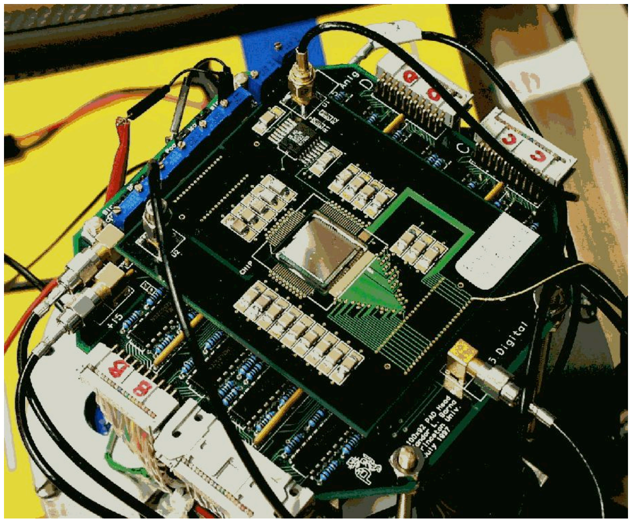


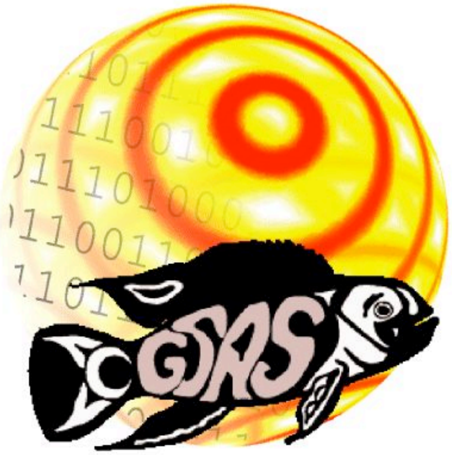
Fig. 3. Thin, needle-like crystals of β-2-adrenergic receptor. The investigators used a 5-µm-diameter beam to target the best part of the crystal, maximized the diffraction/background by only hitting the crystal and not the surrounding mother liquor, and walked along the crystal collecting partial data sets, which were merged to solve the structure. Beam sizes are indicated in the crystal to provide a sense of scale. (Courtesy B. Kobilka and W. Weis, Stanford University)

Critically important supporting capabilities

- Detectors
- Optics
- Computing and software
- Additional laboratory space







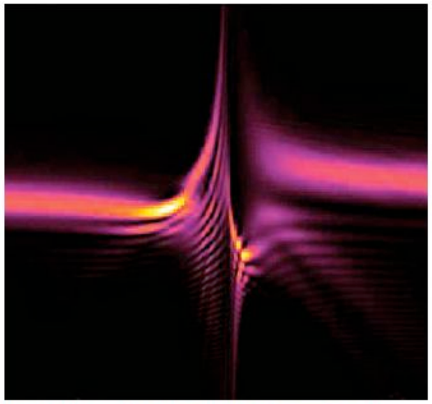
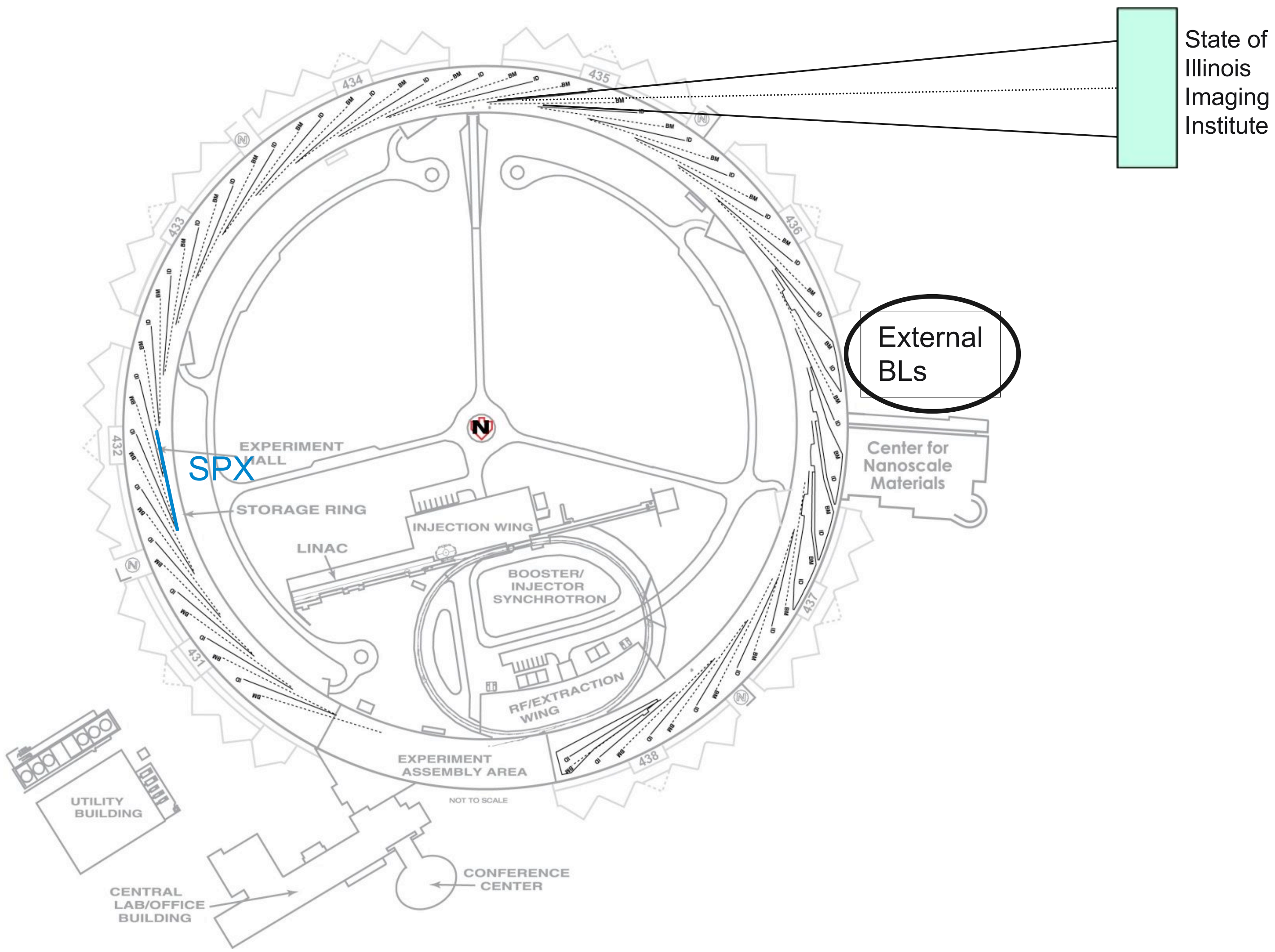


Fig. 3. Simulation of the nanodiffraction topograph arising from a highly strained silicon structure [21]. (© 2008 American Institute of Physics)

Possible configuration for long or complex beamlines

Very few existing BLs must move



Conclusions and next steps

- We have been asked to prepare a proposal for CD-0, due by the end of May
  - Hope to get CD-0 by the end of the summer
- Estimated cost of Renewal (with contingency) $400M
- Looking beyond CD-0, anticipating the next steps:
  - during the summer we will initiate further work on components of this vision
  - will identify contacts for each WBS element (e.g. ”Imaging and coherence”) to coordinate
- SAC is meeting October, at which point we hope to begin the formal planning for the project, including the components of the CDR which will be due in FY2010
- Project funding could begin in FY2011